Poster

Navigation through high-dimensional chemical space: discovery of two Ba-Y silicates

Nataliia Hulai[1], Marco Zanella[1], Craig M. Robertson[1], Daniel Ritchie[1,2], Manel Sonni[1], Matthew A. Wright[1], Jon A. Newnham[1], Cara J. Hawkins[1], Jayne Whitworth[1], Bhupendra Mali[1], Hongjun Niu[1], Matthew S. Dyer[1], Christopher M. Collins[1,2], Luke M. Daniels[1], John B. Claridge[1], Matthew J. Rosseinsky[1,2]

[1]Department of Chemistry, University of Liverpool, Materials Innovation Factory, 51 Oxford Street, Liverpool, L7 3NY, UK,
[2]Leverhulme Research Centre for Functional Materials Design, Materials Innovation Factory, 51 Oxford Street, University of Liverpool, Liverpool L7 3NY, UK.

Nataliia.Hulai@liverpool.ac.uk

Despite recent advances in automation and integrations of artificial intelligence in the exploration process, discovery of new materials still remains a challenging task. However, it has been already proven that the best outcome arises from augmentation of traditional experimental routines with the techniques and tools which enable more efficient exploration of chemical spaces, identification of new phases, and their characterization [1].

In a present study, we showcase how newly developed tools and techniques can be integrated in the traditional experimental route with an example of the solid-state chemistry. During an exploration of the BaO-Y_2O_3-SiO_2-RuO_2 phase field, two new phases were isolated using two complementary experimental routes. The schematic description of the used routine is shown in Figure 1. The first phase $Ba_5Y_{13}[SiO_4]_8O_{8.5}$ (A) was isolated using iterative diffraction-elemental analysis routine. The second phase $Ba_3Y_2[Si_2O_7]_2$ (B) is located in a SiO_2-rich corner of the compositional diagram close to a competing glass field which prevented definitive use of elemental analysis. Due to challenging experimental synthetic conditions, isolation of this phase was guided by a computational tool Probabilistic Isolation of Crystalline Inorganic Phases. The polycrystalline samples were analysed and the crystal structures were solved based on multiple source diffraction techniques. Combination of these complementary routines enabled discovery of phases in already well-explored chemical space. The unveiled structural peculiarities expand knowledge on the crystal chemistry of Ba-Y silicate compounds. Based on physical properties, phase A was assessed to be a prospective phosphor host.

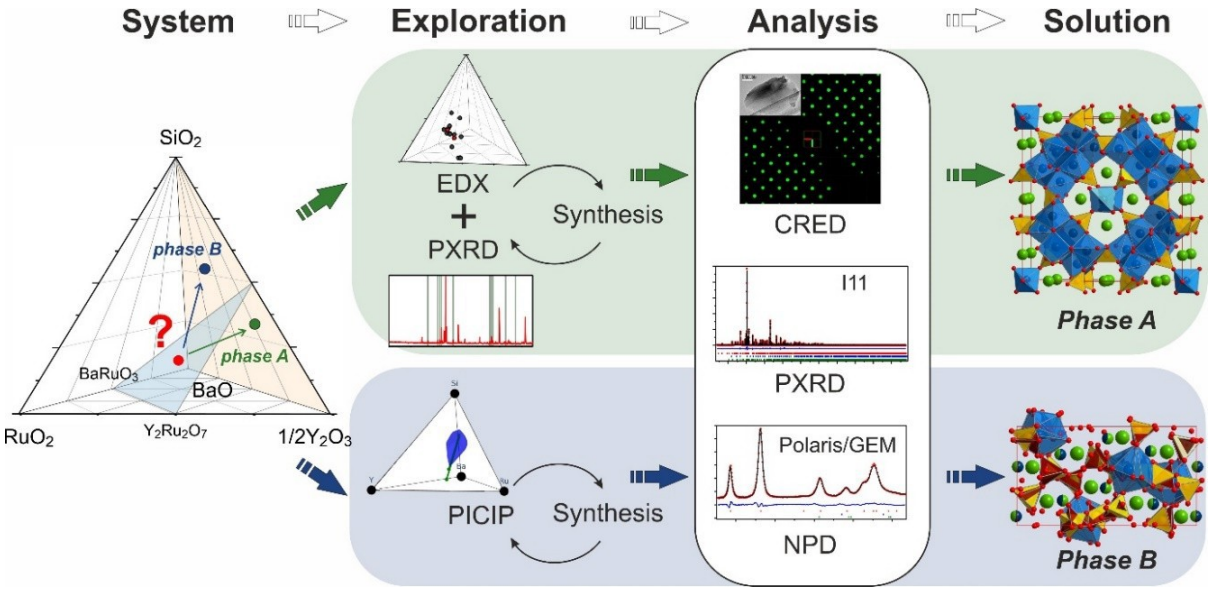

Figure 1. Schematic description of the exploration of the BaO-Y_2O_3-SiO_2-RuO_2 chemical space

[1] Mroz A.M., Posligua V., Tarzia A., Wolpert E.H., Jelfs K.E., *J. Am. Chem. Soc.* **2022**, *144*, 18730.